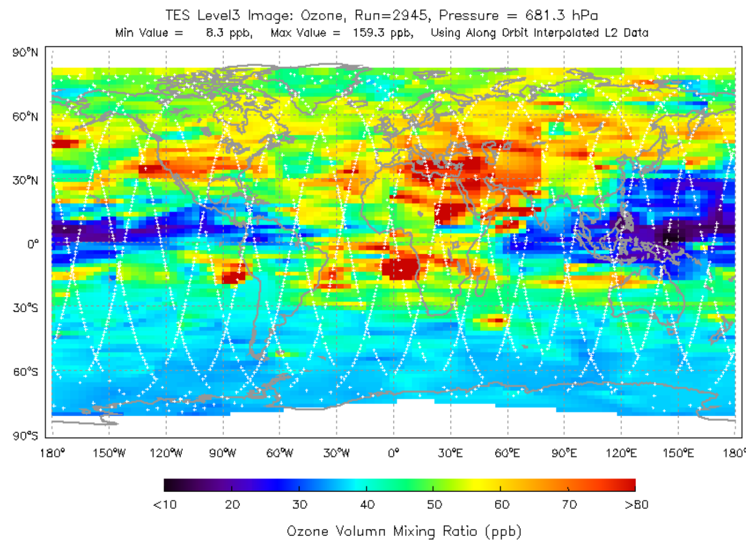
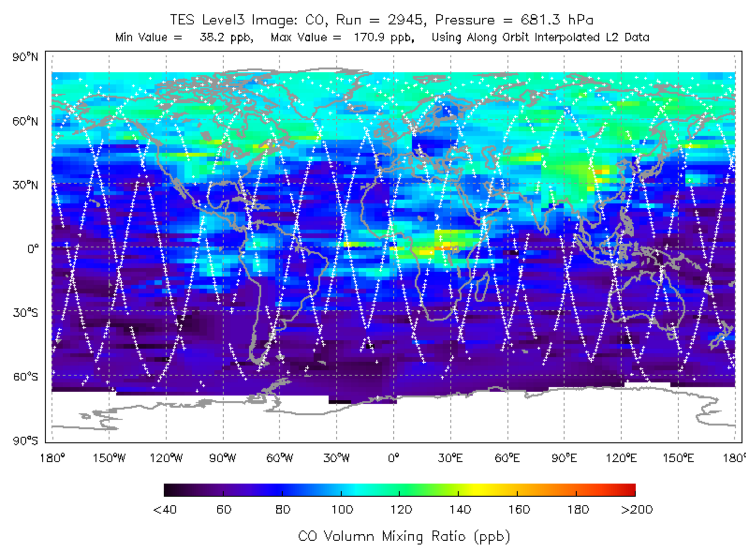
TROPOSPHERIC EMISSION SPECTROMETER

TES L2 Data User's Guide





Version 1.00
April 11, 2006

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

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Table of Contents

1 Scope of this document

This document will provide an overview of the TES instrument and the Level 2 (L2) volume mixing ratio (vmr) and temperature profile data that it measures. The document should provide an investigator the information necessary to successfully use TES data for scientific studies.

This document should be considered an overview of the TES instrument and data, but many additional sources of information are available. The primary sources of information about TES data and data product files are the TES Data Product Specification (DPS) Documents [Lewicki, 2005]. The DPS documents provide extensive information about the data product file content, file sizes and obtaining TES data. The TES L2 Algorithm Theoretical Basis Document (Osterman, *et al.* 2004) provides information about the TES L2 retrieval algorithm, support products and forward model. TES data products are currently undergoing an extensive validation of their scientific quality and an overview of initial validation results is provided in section 8. More information about validation of the TES L2 products can be found in the TES Validation Report (Osterman, *et al.* 2005). There are several other documents that provide important information about TES and they are listed according to subject in the references section (9).

Users of TES data are encouraged to contact the TES science team for further guidance on successfully applying and interpreting the data products. Contact information for TES team members is available at the TES web page (http://tes.jpl.nasa.gov/team/index.cfm).

2 An overview of the TES instrument

2.1 Instrument description

The Tropospheric Emission Spectrometer (TES) on EOS-Aura was designed to measure the global, vertical distribution of tropospheric ozone and ozone precursors such as carbon monoxide (Beer, et al., 2001; Beer, 2006). TES is a nadir and limb viewing infrared Fourier transform spectrometer (FTS) (http://tes.jpl.nasa.gov/mission/instrument.cfm). The TES spectral range is from 650 to 3250 cm^{-1}. The apodized resolution for standard TES spectra is 0.10 cm-1, however, finer resolution (0.025 cm^{-1}) is available for special observations. The footprint of each nadir observation is 5 km by 8 km, averaged over detectors. Limb observations (each detector) have a projection around 2.3 km x 23 km (vertical x horizontal).

TES is on the EOS-Aura platform (http://aura.gsfc.nasa.gov/) in a near-polar, sun-synchronous, 705 km altitude orbit. The ascending node equator crossings are near 1:45 pm local solar time.

2.2 TES observation modes

TES makes routine observations in a mode referred to as the "global survey". A global survey is run every other day on a predefined schedule and collects 16 orbits (~26 hours) of continuous data. Each obit consists of a series of repetitive units referred to as a sequence. A sequence is further broken down into scans. Global surveys are always started at the minimum latitude of an Aura orbit.

The at-launch version of the global survey consisted of 1152 sequences (72 per orbit). Each sequence was made up of 2 calibration scans, 2 nadir viewing scans and 3 limb scans. The two nadir scans for this version of the global survey were acquired at the same location on the spacecraft ground track and the radiances averaged, leading to a single TES L2 profile. The along-track distance between the successive nadir scan locations is ~544 km for this version of the global survey.

On May 25, 2005 the global survey was modified to conserve instrument life. The three limb scans were eliminated from the sequences and replaced by an additional nadir scan. In this version the three nadir scans are acquired at locations equally spaced along the spacecraft ground track. The spacecraft ground track distance between successive nadir observations is ~182 km. The radiances of individual scans are not averaged for data acquired with this version of the global survey. As with the original global survey there are 1152 sequences per global survey and with the additional nadir scans there is a maximum of 3456 profiles for these global surveys.

On January 10, 2006 the last sequence in each orbit was replaced with an instrument maintenance operation. For this version of the global survey there are 1136 sequences per global survey (71 per orbit), meaning a maximum of 3408 L2 profiles. The along-track distance between successive nadir observations was unchanged.

Observations are sometimes scheduled on non-global survey days. In general these are measurements for validation or with highly focused science objectives. These non-global survey measurements are referred to as "special observations". Five special observation scenarios have been used to date and are summarized in Table 1.

Table 1: Description of TES special observation modes.

Name	Pointing	Sequences	Scans per Sequence	Distance Between Scans	Comments
Step and Stare (prior to Jan 1, 2006)	Nadir	1	125	45 km	Continuous along-track nadir views, ~50 degrees of latitude.
Step and Stare (after Jan 1, 2006)	Nadir	6	25	40 km	Continuous along-track nadir views, ~45 degrees of latitude.
Transect	Near Nadir	1	40	12 km	Hi density along-track, near nadir views.
Stare	Near Nadir	1	32	0 km	All measurements at a single location.

Name	Pointing	Sequences	Scans per Sequence	Distance Between Scans	Comments
Limb Only	Limb	1	62	45 km	Continuous along-track limb views, 25 degrees of latitude.
Limb HIRDLS	Limb	142	3	182 km	2 orbits of continuous limb measurements for HIRDLS comparison

2.2.1 2.3 TES Scan Identification Nomenclature

Each TES scan is uniquely identified by a set of three numbers call the run ID, the sequence ID and the scan ID. Each major unit of observation is assigned a unique run ID. Run IDs increase sequentially with time. The first on-orbit run ID is 2000. The seq ID is assigned to repetitive units of measurements within a run. They start at 1 and are automatically incremented serially by the TES flight software. The scan ID is also incremented by the flight software each time a scan is performed. When the sequence is set to 1 the scan ID is set to 0.

3 Where to obtain TES data

The primary location to obtain the TES data products is the Langley Atmospheric Science Data Center (ASDC) which can be found at http://eosweb.larc.nasa.gov/ . The site contains all TES data as well as supporting documentation. All TES data products are in HDF 5 format and completely documented in the TES Data Product Specification documents referenced in Section 9.

4 An overview of TES L2 data products

4.1 File formats and data versions

Each time TES makes a set of measurements, that data set is assigned an identification number (referred to as a "run ID"). A calendar of the TES run IDs for global surveys and a list of all TES run IDs (including observation data, time and date) can be found at http://tes.jpl.nasa.gov/science/dataCalendar.cfm .

Information about the TES data file content and format versioning can be found in the L2 product filenames. There are currently three different versions of TES L2 data products publicly available. It is currently planned that the entire TES L2 data product set shall be processed with the latest software release by approximately October 1, 2006. In the meantime it is important to understand the differences in the data versions and file formats.

Information about the version of TES data is provided in the filename of the L2 products. Table 2 provides an explanation of the TES versions strings and more information about the different data versions is provided in the following sections. A change in the format number corresponds to changes in the fields available or minor bug fixes. A change in content number means a major change in the science content of certain fields in the data products.

The version F03_02 data contains significant upgrades to the science content in the data products and is often referred to as V02 TES data.

Table 2: Description of the TES L2 data product version labels.

TES Version String	Format Version	Science Content Version	Description
F01_F01	1	1	The first publicly released L2 data
F02_01	2	1	Bug fixes and additional fields
F03_02	3	2	Some additional fields but major upgrade to scientific quality of data.

4.2 TES Standard L2 Products

Currently the TES data products available for any given run ID are listed in Table 3. The products are separated by species with an ancillary file providing additional data fields applicable to all species. A description of the contents of the product files, information on the Earth Science Data Type names and file organization can be found in the TES DPS document [Lewicki, 2005]. TES limb products will become available in the next release of data. The methane products should not be used at this time.

Table 3: Description of the TES L2 data product files currently available.

TES L2 Standard Data Product	TES View Mode	Description
Ozone	Nadir	TES nadir ozone profiles and some geolocation information
Temperature	Nadir	TES nadir atmospheric temperature profiles and some geolocation information.
Water	Nadir	TES nadir atmospheric temperature profiles and some geolocation information
Carbon Monoxide	Nadir	TES nadir carbon monoxide profiles and some geolocation information
Methane	Nadir	TES nadir methane profiles and some geolocation information
Ancillary	Nadir	Additional data fields necessary for using retrieved profiles.

TES retrieves surface temperature and it is reported in each species file, however the value in the atmospheric temperature file is the one that should be used for scientific analysis.

The TES L2 Data Products are provided in files separated out by the atmospherics species being measured. An example file name is:

TES-Aura_L2-O3-Nadir_r000002945_F01_01.he5

This particular file contains TES nadir measurements of ozone for run ID 2945 (000002945). The data version number is provided after the "F" in the filename. Additionally there are data files with additional (ancillary) data that are important for working with TES data. These ancillary files can be used with any species data file and contains the string "Anc" in the filename.

4.3 TES version F03_02 data

This is the latest version of the TES data that contains significant improvements in scientific data quality over previous versions. It is possible that a data user may find references to TES data releases with a number attached. This particular version of the data products were created using the "Release 9" or "R9" software and any references to R9 data in TES documentation are consistent with F03_02. It is also referred to as TES data version V02.

This version of the L2 data has been retrieved from L1B products that feature a significantly improved radiance calibration (Sarkissian *et al.,* December 2005). It represents the best retrieval possible currently available for the L2 products.

4.3.1 Known issues or advisories for the TES version F03_02 data

The TES team has determined a few instances where the most recent data product version should not be used for scientific analysis or used with caution. These are listed below and should be fixed in a future version of the TES data.

- Potentially large retrieval errors in the lowest layers of the ozone profile for nighttime (descending orbit path) target scenes over land. In some of these night/land cases, a condition can exist where the lowest levels of the atmospheric temperature profile are sufficiently warmer than the surface to create a layer of relatively high thermal contrast. This creates enhanced sensitivity to ozone in emission compared to the ozone in absorption in the layers above it; however, the modeled radiance for the layers in emission would tend to cancel the radiance for the adjacent layer in absorption. The retrieval constraints were not developed for this condition and it can lead to a solution of artificially high ozone.
- Emissivity retrievals over desert scenes with strong silicate features can be problematic. Version F03_02 contains an additional land type for our emissivity initial guess, "alluvial sand". This improved the TES retrieved emissivity for target scenes over the Sahara desert. This land type is currently only for the Sahara desert region in Africa. Consequently the ozone retrievals in the Sahara desert have improved over previous data versions, but the user should be aware that there may be remaining retrieval difficulties for surfaces with high

reflectance due to silicate features, which we observe in the Sahara desert, parts of central Australia, and desert regions in Asia.

- Methane products are reported, but should not be (in nearly all cases) used for scientific analysis. Ways of improving the methane product are being tested and should be included in a future version of the TES data.
- Fill value for data product files is -999.
- Surface emissivity is not retrieved over ocean and should be fill values in these cases.
- The field TotalColumnDensityInitial contains fill values.
- The nadir geolocation field DominantSurfaceType contains fill values.
- The ancillary file nadir fields OzoneTroposphericColumn, OzoneTroposphericColumnError and OzoneTroposphericColumnInitial contain fill values.
- The units for the constraint vector (ConstraintVector) is incorrectly written to the product file, the units should be 'ln(vmr) or K' not 'vmr or K'.
- Data is not reported for failed target scenes. Consequently, file sizes will differ between runs.

4.3.2 Known issues or advisories for the TES version F02_01 data

This version of the TES L2 retrieval software was not used for long and there are few TES run IDs processed to this combination of format and data quality. Most importantly these data were not processed using the current L1B radiance calibration. These data were processed with the software version "Release 8" or "R8" and data users may see the version F02_01 data referred to as R8.

- These data contain any advisories seen in the version F03_02 data (Section 4.3.1)
- There are problems retrieving surface emissivity over certain types of desert. This is particularly true over the Sahara regions of Africa, possibly central Australia and parts of Asia. These data should be used with caution.
- There is limited information about the cloud or emissivity retrievals included in the data products files (more information in Section 6.2).
- There is limited information about data quality in this version of the product files.
- Run IDs processed with this version contain no limb retrieval information.

4.3.3 Known issues or advisories for the TES version F01_01 data

These were the first TES L2 data products made publicly available. These data were not processed using the current L1B radiance calibration and contains a few processing issues that were resolved for later versions. These data were processed with the software version "Release 7" or "R7" and data users may see the version F01_01 data referred to as R7. It is also referred to as TES data version V01.

- These data contain any advisories included for the version F03_02 data
- These data contain any advisories included for the version F02_01 data
- This data have a problem with retrievals over land. There is a software bug that causes problems with high altitude scenes. Scenes with a surface pressure of ~800 hPa or greater are not affected by this bug. High altitude scenes (< 800 hPa) should not be used for this data version.
- There is no information about the cloud or emissivity retrievals included in the data products files.
- There is very limited information about the data quality in the product files.
- Surface temperature retrievals can be problematic due to a software issue.
- Run IDs processed with this version contain no limb retrieval information.
- The Pressure array contains standard pressures for levels below the surface. These should be fill values. The user is advised to look at another field, such as vmr or Altitude, to determine the index of the surface, which is at the first non-fill value.
- Surface temperature and its error are reported from the last step it was retrieved. It should be reported from the step retrieving it with atmospheric temperature, water and ozone. This results in small errors in the reported surface temperatures, and unreliable reported surface temperature errors.
- The data field "SpeciesRetrievalConverged" is underreported due to convergence criteria that are currently set too strictly.
- The data field "LandSurfaceEmissivity" is incorrectly filled in (by initial guess values) for ocean scenes and should be ignored for these scenes.
- The following field is obsolete and contains fill: CloudTopHeight.
- The data field "CloudTopPressure" is sometimes reported as a value greater than the surface pressure. These locations should be interpreted as being cloud-free.

5 TES data quality information

The quality control information provided along with the TES L2 data products has been improved with each data release. The best way to filter data by quality varies for each release and is described below.

5.1 Data quality information for version F03_02 TES data

The TES retrieval process is non-linear and has the potential to not converge, or converge to a non-global minimum. By studying a larger number of retrievals and comparing results with two different initial conditions, a set of quality flags have been developed and tested that reject about 74% of our bad retrievals and keep about 80% of the "good" retrievals for ozone and temperature. The use of quality flags for other species the filtering percentages are less quantified but should be of a similar order.

A set of quality sub-flags have been developed and are described in the tables below, taken together they make up the "master" quality flag (SpeciesRetrievalQuality). When this flag is set to a value of "1", the data is considered to be of good quality. The master quality flag has been developed for the ozone and temperature retrievals and should not be used for other atmospheric species retrieved by TES. All the numeric values for the quantities used as sub-flags are included in the version F03_02 data files. The thresholds for the ozone and temperature master flags are included in Table 4, while recommended values for carbon monoxide (Table 5) and water (Table 6) are also provided below.

Since all the quality control fields are included in the data products files, less stringent quality flags (or fewer flags) could be used if the user wants more of the good cases left in the pool, realizing that more bad cases will also be included. Note that when a flag is set to -999, such as SurfaceEmissMean_QA for ocean scenes, it does not influence the master quality flag.

We retrieve atmospheric parameters in the following steps (0) Cloud detection and possible cloud initial guess refinement (1) T_{ATM}-H_2O-O_3, (2) H_2O, (3) CO, (4) CH_4. If step (2) does not complete, then the water is reported from step (1) rather than step (2). The user can tell when this occurs because the quality flag CloudVariability_QA (among others) is set to a value different from -999. When this occurs, the user should use the "master" quality flag (SpeciesRetrievalQuality) for H_2O quality. Otherwise, the cutoffs in Table (3) should be used for H_2O quality.

In addition, the threshold for the RadianceResidualMean quality flag for water is set to tight and will be updated in the next release of the data. When using the F03_02 data the user can use all data in which the absolute value of the RadianceResidualMean flag is less than 0.3 and the RadianceResidualRMS is less than 1.4.

Table 4: Values for the ten quality "sub-flags" that, taken together, define the master quality flag for ozone and temperature. If all of these criteria are met for an ozone or temperature profile, the master quality flag is set to "1" (good).

Flag	Description	Minimum Value	Maximum Value
AverageCloudEffOpticalDepth	The average Cloud optical depth between 975-1300 cm^{-1}. When the optical depth is large, the data results seem to have non-linearity issues.	0	50
CloudVariability_QA	The Cloud OD variability over the retrieved frequencies, scaled by the expected cloud OD error. When the variability is too large, it suggests that the clouds do not exhibit the expected spectral smoothness.	0	2
SurfaceEmissMean_QA	The retrieved emissivity bias	-0.1	0.1

Flag	Description	Minimum Value	Maximum Value
	compared to the *a priori*. If the bias large, it is flagged. Note, when emissivity is not retrieved (over ocean or for limb viewing mode) this is set to -999.		
KDotDL_QA	This looks for signal remaining in the radiance residual by calculating the correlation of each Jacobian with the radiance residual, normalized by the NESR. The max correlation of all the retrieved parameters is reported.	-0.17	0.17
LDotDL_QA	This looks for signal remaining in the radiance residual by calculating the correlation of the radiance with the radiance residual, normalized by the NESR.	-0.17	0.17
CloudTopPressure	The cloud top pressure. If this is smaller than 90 mb, it is suspect.	90	1300
SurfaceTempvsAtmTemp_QA	Comparison between the boundary layer atmospheric temperature with the surface temperature. When this is very large, the retrieval is suspect. However, the threshold is the same for land and ocean scenes, so a user of ocean scene results may wish to tighten the allowed range. Note when atmospheric temperature and surface temperature are not retrieved this is set to fill.	-25	25
SurfaceTempvsApriori_QA	Comparison between the retrieved and initial surface temperatures. The metrology for surface temperature is expected to be accurate to about 2K. When difference between the result and the initial guess for surface temperature is much larger than	-8	8

Flag	Description	Minimum Value	Maximum Value
	this, the retrieval is suspect. Note when surface temperature is not retrieved this is set to -999.		
RadianceResidualMean	The mean of the difference between observed and fit radiance normalized by the NESR.	-0.1	0.1
RadianceResidualRMS	The rms of the difference between observed and fit radiance normalized by the NESR. Note that this shows a latitudinal variation, peaking in the tropics, for the TATM-H2O-O3 step, but shows no latitudinal variability for CO or H2O-HDO steps.	0.5	1.75

Table 5: Recommended ranges for TES L2 quality flags for carbon monoxide.

Flag	Minimum Value	Maximum Value
AverageCloudEffOpticalDepth	0	50
CloudVariability_QA	0	2
SurfaceEmissMean_QA	-0.2	0.2
KDotDL_QA	-0.45	0.45
LDotDL_QA	-0.45	0.45
CloudTopPressure	90	1300
SurfaceTempvsApriori_QA	-8	8
RadianceResidualMean	-0.5	0.5
RadianceResidualRMS	0.5	1.1

Table 6: Recommended ranges for TES L2 quality flags for water vapor.

Flag	Minimum Value	Maximum Value
KDotDL_QA	-0.45	0.45
LDotDL_QA	-0.45	0.45
RadianceResidualMean	-0.3	0.3
RadianceResidualRMS	0.5	1.4

5.2 Data quality information for version F02_01 TES data

This version of the data products contains a version of the master quality flag. This flag was optimized to the ozone and temperature retrievals. The values for the sub-flags that went into defining the master quality flag are given in Table 7. The version F02_01 data products contain the master quality flag, but not the complete set of the sub-flags, so it will not be possible for a user to create customized quality flags with this version of the data.

Table 7: The values for the TES quality sub-flags that go into defining the master quality flag for ozone and temperature for version F02_01. If all of these criteria are met for an ozone or temperature profile, the master quality flag is set to "1" (good).

Flag	Minimum Value	Maximum Value
AverageCloudEffOpticalDepth	0	50
CloudVariability_QA	0	2
SurfaceEmissMean_QA	-0.1	0.1
KDotDL_QA	-0.17	0.17
LDotDL_QA	-0.17	0.17
CloudTopPressure	90	1300
SurfaceTempvsAtmTemp_QA	-25	25
SurfaceTempvsApriori_QA	-8	8
RadianceResidualMean	-0.1	0.1
RadianceResidualRMS	0.5	1.5

5.3 Data quality information for version F01_01 TES data

This version of the products has limited quality control information. The data can be filtered on two values, the radiance residual mean (RadianceResidualMean) which should be less than 1.5 for this version and the radiance residual RMS (RadianceResidualRMS) which should be less than 0.1. This combination of data quality fields should be used for filtering the data for all retrieved species in this version of the TES data.

6 TES algorithm for inclusion of clouds in L2 retrievals

Clouds are a significant interferent when estimating the distribution of atmospheric trace gases using infrared remote sensing measurements. We have implemented a single-layer non-scattering cloud into our radiative transfer, parameterized as a non-scattering frequency-dependent effective optical depth distribution and a cloud height. These cloud parameters are estimated from spectral data in conjunction with surface temperature, emissivity, atmospheric temperature, and trace gases. From simulations and TES observation comparisons to model fields and atmospheric measurements from AIRS and TOMS, we show that this approach produces accurate estimates and error characterization of atmospheric trace gases for a wide variety of cloud conditions, and introduces no biases into TES estimates of temperature and trace gases for the cases studied. (Kulawik *et al*., 2006).

A cloud in the observed atmosphere will reduce sensitivities to trace gases below the cloud, for example an optical depth of 1.0 reduces sensitivity below the cloud to 1/3 of the clear-sky sensitivity (Kulawik *et al*., 2006). The sensitivity reduction due to the clouds and all other effects is contained in the averaging kernel, which is provided in the product for each species for each target scene. The averaging kernel describes the sensitivity of the retrieval to the true state (described in more detail in the next section).

6.1 Effective cloud property information available in the F03_02 data

The cloud property information provided in this version of the TES data products is the most extensive. The most important cloud related fields are CloudTopPressure, CloudTopPressureError, CloudEffectiveOpticalDepth, CloudEffectiveOpticalDepthError, and AverageCloudEffOpticalDepth. Cloud effective optical depth and cloud optical depth error fields are discussed in more detail below.

CloudTopPressure can contain fill data if the retrieved cloud top pressure was below the surface (as happens in some very low optical depth cases). It should be noted also that the CloudTopPressure error is in log space.

The AverageCloudEffOpticalDepth does not contain useable data in this version of the data products.

6.2 Effective cloud property information available in the F02_01 data

The version of the data products contains fields: CloudTopPressure, CloudTopPressureError, CloudEffectiveOpticalDepth, and CloudEffectiveOpticalDepthError.

CloudTopPressure can contain fill data if the retrieved cloud top pressure was below the surface (as happens in some very low optical depth cases). It should be noted also that the CloudTopPressure error is in log space.

The AverageCloudEffOpticalDepth does not contain useable data in this version of the data products.

6.3 Effective cloud property information available in the F02_01 data

This version of the data products contains only the fields CloudTopPressure and CloudTopHeight.

There is no cloud optical depth information reported in this version.

The CloudTopHeight field contains fill data.

6.4 Discussion of CloudEffectiveOpticalDepth and CloudEffectiveOpticalDepthError:

The CloudEffectiveOpticalDepth and error are retrieved on a fixed frequency grid.

Table xx shows the frequencies that are retrieved and the corresponding species. The cloud top pressure is retrieved whenever the effective optical depth is retrieved. Note that the sensitivity to clouds is not the same at all frequencies, and some will be more influenced by the *a priori.* The *a priori* is not in the data product file, and since the errors are not reported correctly, it is suggested that the user focus on the optical depths reported at 1000 and 1250 cm-1, where there is good sensitivity.

Frequency	F02_01 and F03_02
600	Not retrieved
650	Not retrieved
700	Not retrieved
750	Not retrieved
800	Not retrieved
850	Not retrieved
900	Not retrieved
950	Not retrieved
975	TATM, H2O, O3
1000	TATM, H2O, O3
1025	TATM, H2O, O3
1050	TATM, H2O, O3
1075	TATM, H2O, O3
1100	TATM, H2O, O3
1150	TATM, H2O, O3
1200	TATM, H2O, O3
1250	TATM, H2O, O3
1300	TATM, H2O, O3, then CH4
1350	TATM, H2O, O3, then CH4
1400	Not retrieved
1900	Not retrieved
2000	CO
2100	CO
2200	CO
2250	Not retrieved

Table 8: A list of atmospheric species that TES retrieves as a function of frequency.

Currently, all of the product files report the effective optical depth from all retrieval steps. Thus, the H2O product file will report effective optical depths for 2000-2200 cm-1, even though that is not retrieved with that species.

The effective cloud optical depth errors are not correct in this data version, so the CloudEffectiveOpticalDepthError field should not be used.

From other analysis, we find that the effective optical depth have large uncertainty for effective optical depths less than a few tenths and greater than 2 or so. The small optical depths indicate that a cloud is present, but provide little information on the actual effective optical depth.

6.5 Discussion of CloudTopPressure and CloudTopPressureError:

Analysis of the cloud top pressure and cloud optical depths reveals that the cloud top pressure errors are low when the cloud optical depth becomes larger (between a few tenths to ten). For very larger optical depths, which likely correspond to low radiance cases, the cloud top pressure error becomes large again.

7 TES Data for Assimilation, Inverse modeling and intercomparison

7.1 Introduction

The TES retrieval algorithm estimates an atmospheric profile by simultaneously minimizing the difference between observed and model spectral radiances subject to the constraint that the solution is consistent with an *a priori* mean and covariance. Consequently, the retrieved profile includes contributions from observations with random and systematic errors and from the prior. These contributions must be properly characterized in order to use TES retrievals in data assimilation, inverse modeling, averaging, and intercomparison with other measurements. All TES retrievals report measurement and systematic error covariances along with averaging kernel and *a priori* vector. We illustrate how to use these TES data with a comparison of TES ozone retrieval to the GEOS-CHEM chemical transport model.

7.1.1 Characterization of TES retrievals and comparisons to models

If the estimate of a profile is spectrally linear with respect to the true state then the retrieval may be written as Rodgers, (2000)

$$\hat{\mathbf{y}}_t^i = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i(\mathbf{y}_t^i - \mathbf{y}_{t,c}^i) + \varepsilon_t^i \qquad (1)$$

where $\hat{\mathbf{y}}_t^i$ is a vector containing the estimated atmospheric state at time t and location i, $\mathbf{y}_{t,c}^i$ is the constraint vector, $\mathbf{y}_t^i$ is the true atmospheric state, $\mathbf{A}_t^i$ is the averaging kernel, and ε_t^i is the observational error (Bowman *et al,* 2006).

The estimated atmospheric state may be include the vertical distribution of atmospheric temperature and traces gases as well as effective cloud and surface properties, e.g. surface temperature and emissivity. For the case of trace gas profiles such as carbon monoxide and ozone, the atmospheric state is cast in the logarithm:

$$\mathbf{y}_t^i = \ln \mathbf{x}_t^i \qquad (2)$$

where $\mathbf{x}_t^i$ is a vector whose elements are the vertical distribution of a trace gas in volume mixing ratio.

A retrieval characterized by the averaging kernel and constraint vector can be used to quantitatively compare model fields and *in situ* measurements directly to TES vertical profiles. If the model fields are defined as

$$\mathbf{y}_t^{i,m} = \mathbf{F}(\mathbf{x}_t, \mathbf{u}_t, t) \qquad (3)$$

where $\mathbf{x}$ is a vector of model fields, $\mathbf{u}$ is a vector of model parameters, e.g. sources and sinks of carbon monoxide, $\mathbf{F}$ is the model operator where the range is defined in terms of the volume mixing ratio for trace gases.

The TES *observation operator* can be written as

$$\mathbf{H}_t(\mathbf{x}_t, \mathbf{u}_t, t) = \mathbf{y}_{t,c}^i + \mathbf{A}_t^i(\ln \mathbf{F}(\mathbf{x}_t, \mathbf{u}_t, t) - \mathbf{y}_{t,c}^i) \qquad (4)$$

The logarithm is not applied to model fields associated with atmospheric temperature and surface quantities. From the standpoint of the model, the observations are now expressed in the standard additive noise model, (Jones *et al*., 2004):

$$\hat{\mathbf{y}}_t^{i,m} = \mathbf{H}(\mathbf{x}_t, \mathbf{u}_t, t) + \varepsilon \qquad (5)$$

The TES observation operator accounts for the bias and resolution of the TES retrieval. Consequently a comparison with TES estimates with a model or *in-situ* data can be described as follows:

$$\hat{\mathbf{y}}_t^i - \hat{\mathbf{y}}_t^{i,m} = \mathbf{A}_t^i(\mathbf{y}_t^i - \ln \mathbf{F}(\mathbf{x}_t, \mathbf{u}_t, t)) + \varepsilon_t^i \qquad (6)$$

The bias in the estimate is removed in the difference. Differences greater than the observational error can be ascribed to differences between the model and the atmospheric state.

The TES ozone retrieval shown in Figure 1was taken from an observation near the island of Sumisu-jima off the coast of Japan on Sept 20, 2004. Figure 3 is the averaging kernel calculated for that retrieval. The green profile was calculated by applying the TES observation operator (Equation (4)) to the GEOS-CHEM model field (2x2.5 degrees). The error bars are calculated from standard deviation of the observational error covariance matrix.

For this retrieval, the sensitivity of the retrieval below 800 mb is reduced due to the presence of clouds. Consequently, the GEOS-Chem model profile at those pressure levels relaxes back to the TES *a priori* after the application of the TES observation operator. However, both the GEOS-Chem model and the TES retrieval indicate elevated amounts of ozone in the upper troposphere. The differences between the TES retrieval and GEOS-Chem model are significantly greater than the known observation errors. Therefore, those differences can be attributed to actual differences between the model and the atmospheric state or currently unknown systematic errors within the retrieval.

7.1.2 Mapping (interpolation) and the averaging kernel

The averaging kernel, an example of which is shown in Figure 2, is the sensitivity of the retrieved profile to changes in the true state and is composed of 3 matrices:

$$\mathbf{A}_t^i = \frac{\partial \hat{\mathbf{y}}_t^i}{\partial \mathbf{y}_t^i} = \mathbf{M}^i \mathbf{G}_z^i \mathbf{K}_y^i$$

where the mapping (interpolation) matrix is defined as

$$\mathbf{y}_t^i = \mathbf{M}\mathbf{z}_t^i, \qquad \mathbf{M} : \mathbf{R}^M \rightarrow \mathbf{R}^N, \;\; M < N \tag{7}$$

and $\mathbf{z}_t^i$ is a reduced state vector, e.g., a profile on a coarser pressure grid. The mapping matrix projects the retrieval coefficients to the forward model levels. This mapping represents a "hard" constraint on the estimated profile, *.i.e.,* restricts the profile to a subspace defined by **M**.

The second matrix is the gain matrix:

$$\mathbf{G}_z^i = \left((\mathbf{K}_y \mathbf{M})^{\mathrm{T}} \mathbf{S}_n^{-1} \mathbf{K}_y \mathbf{M} + \Lambda \right)^{-1} (\mathbf{K}_y \mathbf{M})^{\mathrm{T}} \mathbf{S}_n^{-1} \tag{8}$$

The gain matrix projects the TES observed radiances to the TES estimated profiles based on the, hard constraints **M**, the prior and "soft" constraint Λ. The TES spectral Jacobian is defined as

$$\mathbf{K}_y = \frac{\partial \mathbf{L}}{\partial \mathbf{y}} \tag{9}$$

where **L** is the TES forward model, which encompasses both the radiative transfer and the instrumental lineshape (Clough *et al*, 2006). The averaging kernel is supplied on the forward model pressure grid, which is nominally 87 levels where each level is approximately 1.5 km. The degrees of freedom for signal *(dofs)* for any TES retrieval, which is defined as the trace of the averaging kernel, are significantly less than 87. So, why do we store them on such a fine scale?

- Averaging kernel on a fine pressure scale accommodates a variety of grids, e.g., balloons, tropospheric models, stratospheric models, column trace gas observations
- Averaging kernel can be reduced without loss of information but not vice versa
- Subsequent changes in the retrieval, e.g., changes in **M**, do not change file format.

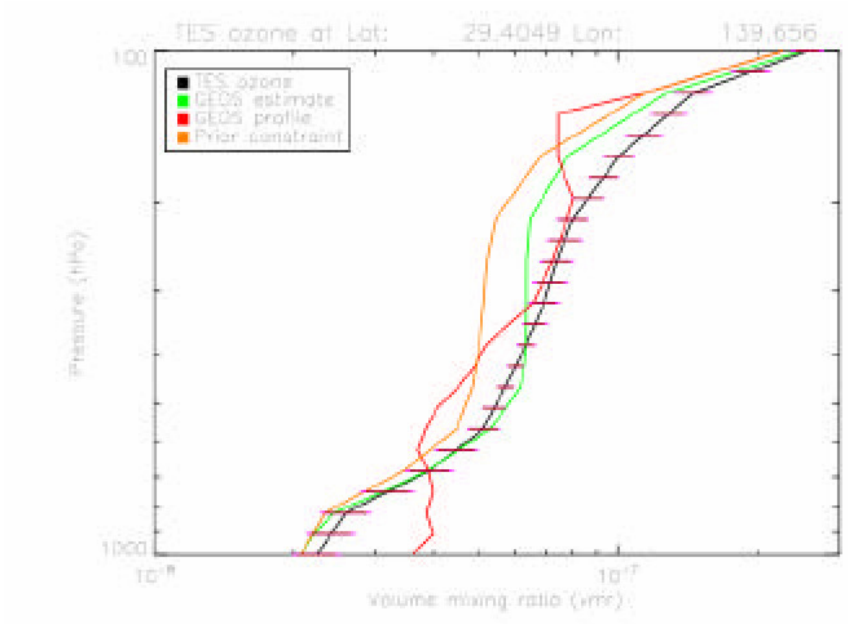

Figure 1: TES nadir ozone retrieval taken from an observation near the island of Sumisu-jima off the coast of Japan on Sept 20, 2004. The green profile was calculated by substituting the natural logarithm of a GEOS-CHEM model field x2.5 degrees) into the model TES retrieval equation.

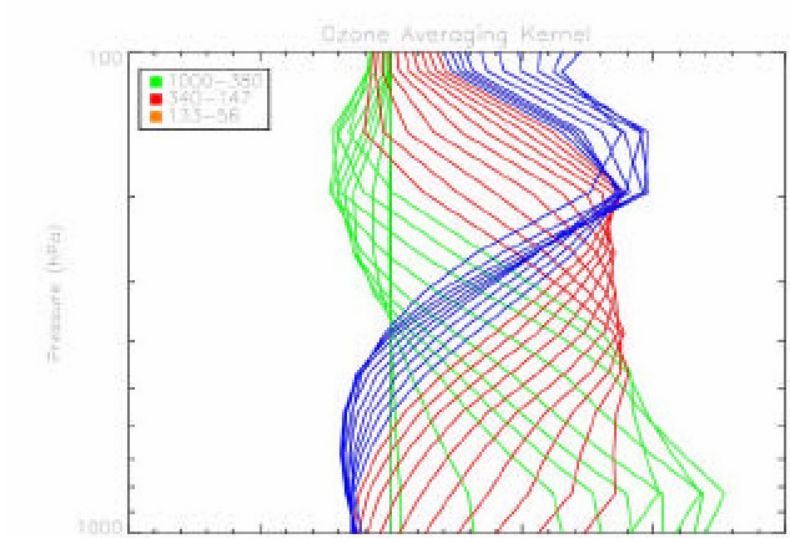

Figure 2: TES ozone logarithm averaging kernel from Sumisu-jima observation. Each vertical distribution is the contribution of the true state to the retrieved state at a given pressure level. The 3 colors indicate three pressure regimes for which the averaging kernels have similar distributions.

7.1.3 Examples of Mapping

There are a variety of ways to implement mapping with TES data depending on the application. In the case of some chemistry and transport models or *in situ* measurements, the atmosphere is discretized on coarser pressure levels. A simple linear interpolation in logarithm of vmr can be used to map these coarser levels to the finer TES levels. This mapping is expressed as:

$$\mathbf{M}_{Trop} : \mathbf{R}^{P} \rightarrow \mathbf{R}^{N} \tag{10}$$

where $P < N$. The model retrieval is then

$$\hat{\mathbf{y}}_{t}^{i,m} = \mathbf{y}_{t,c}^{i} + \mathbf{A}_{t}^{i}(\mathbf{M}_{Trop} \ln \mathbf{F}(\cdot) - \mathbf{y}_{t,c}^{i}) \tag{11}$$

Note that the product of the averaging kernel and the map can be calculated, which results in a smaller composite matrix. Some instruments produce a column quantity based on scaling a fixed climatological profile. These kinds of data can be compared to the TES retrieval by defining a column vector whose entries are the climatological profile. The mapping looks like

$$\mathbf{M}_{c} : \mathbf{R} \rightarrow \mathbf{R}^{N} \tag{12}$$

This quantity is scaled by the quantity α leading to the equivalent profile retrieval

$$\hat{\mathbf{y}}_{t}^{i} = \mathbf{y}_{t,c}^{i} + \mathbf{A}_{t}^{i}(\ln(\mathbf{M}_{c}\alpha) - \mathbf{y}_{t,c}^{i}) \tag{13}$$

This profile can then be compared directly to the TES retrieval.

7.1.4 Conclusions

- TES Level 2 products will include, along with retrievals of atmospheric trace gases, averaging kernels, constraint vectors, and error covariance matrices on the forward model levels
- These tools are critical for comparison of TES retrievals to *in situ* sonde measurements, aircraft and satellite measurements, along with comparison to chemical transport models.
- These techniques enable assimilation systems to properly incorporate TES data by characterizing the constraints and biases used in the retrieval without resorting to expensive and non-linear radiative transfer models

7.2 Using TES data: Comparisons of TES ozone profiles with ozonesondes

The principal source of validation for TES ozone retrievals are comparisons with ozonesonde measurements. In order to make TES-ozonesonde comparisons, we must account for TES measurement sensitivity and the disparities in vertical resolution. This is done by applying the TES averaging kernel and constraint to the ozonesonde profile.

7.2.1 Steps for comparing TES retrieved profiles to sonde data:

1. Pre-process ozonesonde data
   a. Convert pressure, temperature and O3 to hPa, K, vmr (respectively)

b. Remove data at duplicate pressure levels (if any). (Duplicate pressures corrupt the mapping to a common pressure grid.)

c. Append TES initial guess to sonde data in cases where the minimum sonde pressure is > 10 hPa. This is done by scaling the initial guess for O3 and by shifting the intial guess for temperature to the last available sonde values.

d. Interpolate/extrapolate sonde data to a fixed, fine level pressure grid (800 pressure levels, 180 levels per decade pressure, covering 1260 hPa to 0.046 hPa). This ensures a robust mapping procedure since the pressure grids for sondes are variable and non-uniform.

2. Map sonde profile $\mathbf{x}_{sonde}$ to the pressure level grid used for TES profiles (87 levels covering 1212 hPa to 0.1 hPa) using mapping matrix $\mathbf{M}^*$ which is the pseudo-inverse of the matrix M that interpolates from 87 levels to the fine level grid (800 pressure levels) with $\mathbf{M}^* = (\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T$.

3. Apply TES averaging kernel, $\mathbf{A}_{xx}$, and *a priori* constraint $\mathbf{x}_{apriori}$:

$$\mathbf{x}_{sonde}^{est} = \mathbf{x}_{apriori} + \mathbf{A}_{xx}[\mathbf{M}^*\mathbf{x}_{sonde} - \mathbf{x}_{apriori}] \quad (14)$$

to get the estimated profile $\mathbf{x}^{est}{}_{sonde}$ that represents what TES would measure forthe same air sampled by the sonde. For temperature profiles, the **x** is in K. For ozone, water vapor and other trace gases, **x** is the natural log of vmr.

4. Compare to TES profile with respect to the measurement and cross-state error terms. The sum of measurement and cross-state errors is labeled the "observational error", which is provided in TES V002 data products.

The total error estimate is given by:

$$\begin{aligned}
&\mathbf{S}_{\tilde{x}} = \text{(Total error covariance)}\\
&(\mathbf{A}_{xx} - \mathbf{I})\mathbf{S}_a(\mathbf{A}_{xx} - \mathbf{I})^T + \text{ (Smoothing error)}\\
&(\mathbf{A}_{xx_{CS}})\mathbf{S}_a^{x_{cs}x_{cs}}(\mathbf{A}_{xx_{CS}})^T + \text{ (Cross-state error, includes T,H2O)} \quad (15)\\
&\mathbf{M}\mathbf{G}_z\mathbf{S}_n\mathbf{G}_z^T\mathbf{M}^T + \text{ (Measurement error)}\\
&\sum_i \mathbf{M}\mathbf{G}_z\mathbf{K}_\mathbf{b}^i\mathbf{S}_b^i(\mathbf{M}\mathbf{G}_z\mathbf{K}_\mathbf{b}^i)^T \text{ (Systematic errors)}
\end{aligned}$$

where **x** represents the estimated ozone parameters in this case and $\mathbf{M} = \frac{\partial \mathbf{x}}{\partial \mathbf{z}}$ is a linear mapping matrix on pressure levels from retrieval parameters (**z**) to state parameters (**x**). $\mathbf{G}_z$ is the gain matrix, $\mathbf{G}_z = \frac{\partial \mathbf{z}}{\partial \mathbf{F}} = \left(\mathbf{K}_z{}^T\mathbf{S}_n^{-1}\mathbf{K}_z + \Lambda_z\right)^{-1}\mathbf{K}_z{}^T\mathbf{S}_n^{-1}$ where **F** is the forward model radiance, $\mathbf{K}_z$ is the Jacobian matrix, $\mathbf{S}_n$ is the measurement covariance, and Λ_z is the constraint matrix. These give the averaging kernel $\mathbf{A}_{xx} = \mathbf{M}\mathbf{G}_z\mathbf{K}_z\mathbf{M}^{-1}$, which is the sensitivity of the retrieval to the true state. $\mathbf{S_a}$ is the *a priori* covariance (ozone or temperature), $\mathbf{S_a}^{\mathbf{XcsXcs}}$ is the covariance with cross state parameters that are retrieved concurrently. (For ozone, these are atmospheric temperature and water vapor). $\mathbf{S}^i{}_\mathbf{b}$ is the covariance for the ith forward model systematic error, such as spectroscopic uncertainties, and $\mathbf{K}^i{}_\mathbf{b}$ are the jacobian matrices representing the sensitivity of the forward model radiance to these non-retrieved forward model parameters. See Worden, *et al*.[2004] and Bowman *et al.* [2006] for more details on notation and definitions.

8 Overview of current validation status

With the release of the version V02 (F03_02) data, the TES team is working on updating the validation status for each TES standard product. In the case of the V02 TES ozone profiles, some of the work has been completed and a summary of the preliminary validation results for ozone is included in the next section. A summary of the validation status for the other TES products using F01_01 data is also provided.

8.1 Validation Status for TES Products

8.1.1 TES L1B Radiances

At present, TES L1B data products have systematic errors that need to be resolved and/or mitigated. These errors are both target scene dependent and frequency dependent, especially across the 4 TES focal planes that measure different frequency ranges. The TES L1B nadir radiances have an estimated error of around 2% due to systematic errors. Comparisons between TES L1B radiance spectra and those from Aqua-AIRS show that they agree to less than 1K in brightness temperature. Comparisons between TES and the aircraft instrument Scanning HIS show similar results.

8.1.2 Ozone

Statistical analyses for V02 TES retrievals compared to ozonesondes are in progress. Preliminary results from sonde launches timed for the Aura overpass in the tropical Pacific (Galapagos Isl. and Costa Rica) do not indicate a significant bias in the upper troposphere, as was present in V01 data (Worden, *et al*., 2006).

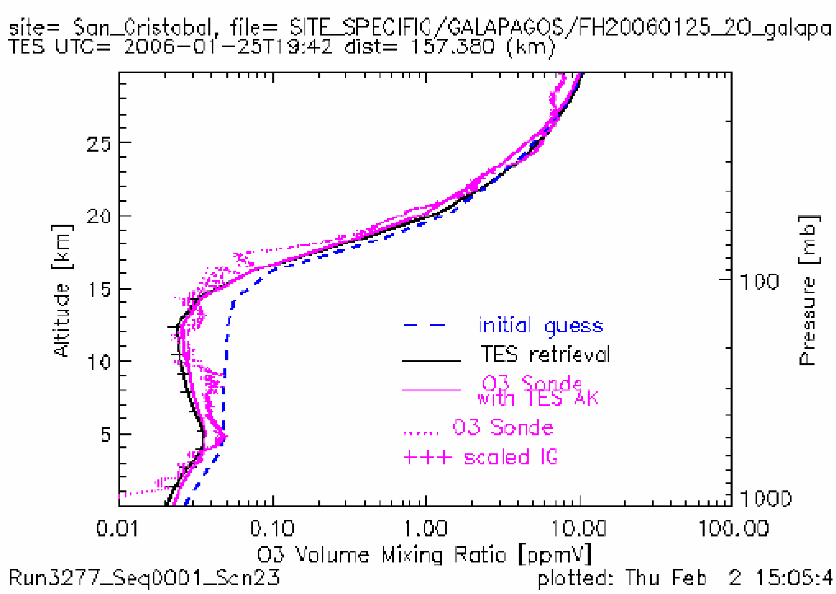

Figure 3: Comparison between TES ozone profile and ozonesonde near San Cristobal on January 25, 2006

8.1.3 Water Vapor

TES total column water vapor is 10% drier than AMSR-E and AIRS. Comparison of the water vapor profiles from TES and AIRS show that most of the difference in the column is accounted for by the 700-900mb layer. Initial comparisons of TES water retrievals show good qualitative agreement.

8.1.4 Atmospheric Temperature

Initial comparisons of AIRS and TES temperature profiles show that the temperature profiles agree to within 2K, The vertical structure of the difference between TES and AIRS profiles is consistent from day to day.

8.1.5 Carbon Monoxide:

Initial comparisons have been carried out between TES carbon monoxide retrievals and those from Terra-MOPITT. The results show that for pressure layers where both instruments are most sensitive, the retrievals agree to within roughly 10%. Comparisons to the aircraft instruments show agreement within the estimated TES retrieval errors.

9 Supporting Documentation

If after using this document, the data user still has further questions the following document provide further information on the TES instrument and data.

Description of the TES instrument can be found in the following publications:

> Beer, R., T. A. Glavich, and D. M. Rider, Tropospheric emission spectrometer for the Earth Observing System's Aura satellite, Applied Optics, 40, 2356-2367, 2001.
>
> Beer, R., TES Scientific Objectives & Approach, Goals & Requirements, Revision 6.0, JPL D-11294, April 14, 1999.

Information on the improved TES L1B radiance calibration is given in the following presentation:

> E. Sarkissian *et al.*, TES Radiometric Assessment, AGU Fall 2005, A41A-0007, December 2005.

A description of the format and contents of the TES data products are provided in the data product specification documents:

> Lewicki, S., TES Science Data Processing Standard and Special Observation Data Products Specifications, Version 9.0, JPL D-22993, December 13, 2005, for public released data, software release 9.
>
> Lewicki, S., TES Science Data Processing Standard and Special Observation Data Products Specifications, Version 8.0, JPL D-22993, July 7, 2005, for public released data, software release 8.

Lewicki, S., TES Science Data Processing Standard and Special Observation Data Products Specifications, Version 7.0, JPL D-22993, March 17, 2005, for public released data, software release 7.

The following list of documents and publications provide information on the algorithms used in producing the data and different aspects of the quality of the TES data products.

Osterman, G.B., Editor, TES Level 2 Algorithm Theoretical Basis Document, Version 1.16, JPL D-16474, June 30, 2004.

Worden, H.M. and Bowman, K.W., TES Level 1B Algorithm Theoretical Basis Document, Version 1.1, JPL-D16479, October, 1999.

S. S. Kulawik, H. Worden, G. Osterman, M. Luo, R. Beer, D. Kinnison, K.W. Bowman, J. Worden, A. Eldering, M. Lampel, T. Steck, C. Rodgers, TES Atmospheric Profile Retrieval Characterization: An orbit of simulated observations, IEEE Trans. Geosci. Remote Sensing, December 8, 2005, accepted.

Kulawik, S.S., J. Worden, A. Eldering, K.W. Bowman, M. Gunson, G. Osterman, L. Zhang, D. Jacob, S.A. Clough, M. Shephard, R. Beer, Implementation of Cloud Retrievals for Tropospheric Emission Spectrometer (TES) Atmospheric Retrievals - part I description and characterization of errors on trace gas retrievals, J. Geophys. Res.-Atmospheres, October 3, 2005, Submitted.

Worden, J.; Sund-Kulawik, S.; Shephard, M. W.; Clough, S. A.; Worden, H.; Bowman, K.; Goldman, A., "Predicted errors of tropospheric emission spectrometer nadir retrievals from spectral window selection", J. Geophys. Res., Vol. 109, No. D9, D09308, 10.1029/2004JD004522, May 15, 2004.

Information on how TES handles clouds in the L2 retrieval process:

Worden, H., Logan, J., and TES team members (2006), Comparisons of Tropospheric Emission Spectrometer (TES) ozone profiles to ozonesondes: methods and results and initial results, submitted to *Journal of Geophysical Research-Atmospheres*, March, 2006

Information on using TES data for data comparisons, assimilation and inverse modeling:

Bowman, K.W., Clive D. Rodgers, Susan Sund-Kulawik, John Worden, Edwin Sarkissian, Greg Osterman, Tilman Steck, Ming Lou, Annmarie Eldering, Mark Shepherd, Helen Worden, Michael Lampel, Shepherd Clough, Pat Brown, Curtis Rinsland, Michael Gunson, Reinhard Beer, "Tropospheric Emission Spectrometer: Retrieval Method and Error Analysis", *IEEE Trans. Geosci. Remote Sensing*, in press, 2006.

Worden, J., S. S. Kulawik, M. Shepard, S. Clough, H. Worden, K. Bowman, and A. Goldman, "Predicted errors of Tropospheric Emission Spectrometer nadir retrievals from spectral window selection," J. Geophys. Res., vol. 109, no. D09308, May 2004.

Worden, H.M., J. A. Logan, J. R. Worden, R. Beer, K. Bowman, S. A. Clough, A. Eldering, B. M. Fisher, M. R. Gunson, R. L. Herman, S. S. Kulawik, M. C. Lampel, M. Luo, I. A. Megretskaia, G. B. Osterman, M.W. Shephard, "TES comparisons to Ozonesonde profiles: Methods and Initial Results", submitted to JGR-Atmospheres, 3/2006.

Information on the initial validation of TES data products:

Osterman, G.B., Editor, TES Validation Report, Version 1.0, JPL D33192, August 15, 2005.

A complete list of TES related documents and publications can be found on the TES "Documents & Links" website http://tes.jpl.nasa.gov/docsLinks/index.cfm .